AmDT/C

ABSTRACT OF THE DISCLOSURE

Methods are provided for searching for stable docking models of biopolymer-ligand molecule complexes, by inputting three-dimensional coordinates for each atom of a biopolymer as well as atomic element, bond-type or covalent bonds and three-dimensional coordinates for each atom of a ligand;

either covering possible docking structures or selecting stable docking structures between the biopolymer and the ligand while changing the conformation of the ligand; and

outputting information about three-dimensional coordinates for each atom of the ligand in one or more stable docking structures including the most stable one relative to the biopolymer; as well as the stability of the docking structures, the binding modes and conformations of the ligand in the structures, wherein matching of distances among dummy atoms and those among either heteroatoms of the ligand or atoms of the ligands are tested, the dummy atoms being preset at the positions of either (a) the heteroatoms that can hydrogen-bond with hydrogen bonding groups in the biopolymer or (b) the atoms of the ligand that interact with functional groups in the biopolymer.